



U.S. Food and Drug Administration
Protecting and Promoting Public Health

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Defining Polymers



What is a Polymer

- A **polymer** is a chemical compound or mixture of compounds consisting of repeating structural units created through a process of **polymerization**.
(Wikipedia)
- **Polymers** are substances containing a large number of structural units joined by the same type of linkage.
- High polymers consists covalent structures many times greater in extent than those existing in simple compounds. (Paul J. Flory)



11238 Definition

- Type of polydisperse substance that contains structural repeating units linked by covalent bonds.

Exclude protein and nucleic acid with defined sequences.

- Polymers
 - Biopolymers (Cellulose, Dextrans, Starches, Heparins)
 - Defined based on the structural repeating units, molecular weight or a property based on molecular weight and the biological source of the polymer.



Polymers

- Semi-synthetic or modified biopolymers
 - Defined based on the biopolymer plus the modification and extent of modification.
 - Fragment modifications
 - Each fragment would be identified by UNII
 - » Fragment would be what is needed when a hydrogen is replaced on the polymer
 - » Methyl fragment for methoxy; Acetyl for acetate
 - Potential site of attachments would be identified
- Synthetic Polymer
 - Type of polymer
 - Homopolymer
 - Crosslinked Homopolymer
 - Copolymer Random
 - Copolymer Block



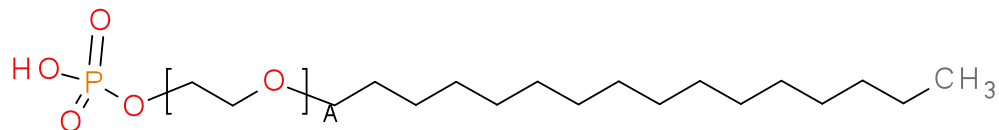
Polymers

- Synthetic Polymer Continued
 - Geometry
 - Linear
 - Branched
 - Network
 - Monomers (Actual Informative or Defining?)
 - Ratio or relative amount of monomers
 - Each monomer would be described with a UNII



Polymers

- Will capture end groups if they are defined or definite.
 - CETETH-10 PHOSPHATE





CETETH-10 PHOSPHATE

xml	version="1.0" encoding="ut
POLYMER	
POLYMER_CLASS	HOMOPOLYMER
POLYMER_GEOMETRY	LINEAR
COPOLYMER_SEQUENCE_TYPE	RANDOM
MONOMER_DESCRIPTION	
NUMBER_OF_MONOMERS	
MONOMER_AMOUNT_TYPE	MONOMERS PER MOLECULE
MONOMER_GROUP	
MONOMER_ID	ETHYLENE OXIDE
MONOMER_NAME	JJH7GNN18P
AMOUNT	
AVERAGE	10
LOW_LIMIT	
HIGH_LIMIT	
UNIT	
NON_NUMERIC_VALUE	
STRUCTURAL_REPEAT_UNIT	
NUMBER_OF_STRUCTURAL_REPEAT_UN	1
STRUCTURAL_REPEAT_UNIT_AMOUNT	UNITS PER MOLECULE
STRUCTURAL_REPEAT_UNIT_GROUP	
ORIENTATION_OF_POLYMERIZAT	HEAD-TAIL
STRUCTURAL_REPEAT_UNIT	A
AMOUNT	
AVERAGE	10
LOW_LIMIT	
HIGH_LIMIT	
UNIT	
NON_NUMERIC_VALUE	
DEGREE_POLYMERIZATION	

HO

- All Heparins have the same structural representation





Enoxaparin Description

POLYMER	
+ POLYMER_CLASS	COPOLYMER
+ POLYMER_GEOMETRY	LINEAR
+ COPOLYMER_SEQUENCE_TYPE	RANDOM
+ MONOMER_DESCRIPTION	
- STRUCTURAL_REPEAT_UNIT	
+ NUMBER_OF_STRUCTURAL_REPEAT_UN	3
+ STRUCTURAL_REPEAT_UNIT_AMOUNT	
- STRUCTURAL_REPEAT_UNIT_GROUP	
+ ORIENTATION_OF_POLYMERIZAT	HEAD-TAIL
+ STRUCTURAL_REPEAT_UNIT	A
+ AMOUNT	
+ DEGREE_POLYMERIZATION	
+ STRUCTURAL_REPEAT_UNIT_GROUP	
+ STRUCTURAL_REPEAT_UNIT_GROUP	
- MOLECULAR_WEIGHT	
+ MOLECULAR_WEIGHT_TYPE	WEIGHT AVERAGE
+ MOLECULAR_WEIGHT_METHOD	HP-SEC
- AMOUNT	
+ AVERAGE	5300
+ LOW_LIMIT	
+ HIGH_LIMIT	
+ UNIT	
+ NON_NUMERIC_VALUE	
- MOLECULAR_WEIGHT	
+ MOLECULAR_WEIGHT_TYPE	NUMBER AVERAGE
+ MOLECULAR_WEIGHT_METHOD	HP-SEC
- AMOUNT	
+ AVERAGE	3800
+ LOW_LIMIT	
+ HIGH_LIMIT	



Enoxaparin Description

POLYMER	
POLYMER_CLASS	COPOLYMER
POLYMER_GEOMETRY	LINEAR
COPOLYMER_SEQUENCE_TYPE	RANDOM
MONOMER_DESCRIPTION	
STRUCTURAL_REPEAT_UNIT	
MOLECULAR_WEIGHT	
MOLECULAR_WEIGHT	
PROPERTY_GROUP	
PROPERTY_TYPE	PHYSICAL
PROPERTY	DEGREE OF SULFATION
SUBSTANCE_NAME	
SUBSTANCE_ID	
AMOUNT_TYPE	PER DISACCHARIDE
AMOUNT	
AVERAGE	2.0
LOW_LIMIT	1.8
HIGH_LIMIT	
UNIT	
NON_NUMERIC_VALUE	
PROPERTY_GROUP	
PROPERTY_TYPE	ENZYMATIC
PROPERTY	ANTI-FACTOR XA/ANTI-FACTOR II RATIO
SUBSTANCE_NAME	
SUBSTANCE_ID	
AMOUNT_TYPE	RATIO
AMOUNT	
AVERAGE	4.3
LOW_LIMIT	3.3
HIGH_LIMIT	5.3
UNIT	
NON_NUMERIC_VALUE	



Enoxaparin Description

POLYMER_CLASS	COPOLYMER
POLYMER_GEOMETRY	LINEAR
COPOLYMER_SEQUENCE_TYPE	RANDOM
MONOMER_DESCRIPTION	
STRUCTURAL_REPEAT_UNIT	
MOLECULAR_WEIGHT	
MOLECULAR_WEIGHT	
PROPERTY_GROUP	
PROPERTY_GROUP	
MODIFICATION_GROUP	
MODIFICATION_TYPE	AGENT
PHYSICAL_MODIFICATION	
STRUCTURAL_MODIFICATION	
AGENT_MODIFICATION	
NUMBER_OF_AGENT_MODIFICATION	2
MODIFICATION	
MODIFICATION_NUMBER	1
AGENT_MODIFICATION_TYPE	ACYLATION
ROLE	
MODIFICATION_AGENT	BENZOYL CHLORIDE
MODIFICATION_AGENT_ID	VTY8706W36
MODIFICATION_PROCESS	
AMOUNT	
MODIFICATION	
MODIFICATION_NUMBER	2
AGENT_MODIFICATION_TYPE	BASE
ROLE	HYDROLYSIS
MODIFICATION_AGENT	
MODIFICATION_AGENT_ID	
MODIFICATION_PROCESS	BETA-ELIMINATION



Enoxaparin Description

tree View XSL Output	
POLYMER	
+ POLYMER_CLASS	COPOLYMER
+ POLYMER_GEOMETRY	LINEAR
+ COPOLYMER_SEQUENCE_TYPE	RANDOM
+ MONOMER_DESCRIPTION	
+ STRUCTURAL_REPEAT_UNIT	
+ MOLECULAR_WEIGHT	
+ MOLECULAR_WEIGHT	
+ PROPERTY_GROUP	
+ PROPERTY_GROUP	
+ MODIFICATION_GROUP	
- SOURCE_MATERIAL	
+ SOURCE_MATERIAL_CLASS	ORGANISM
+ SOURCE_MATERIAL_TYPE	MAMMALIAN
+ SOURCE_MATERIAL_STATE	
+ FAMILY	
+ ORGANISM_NAME_ID	
+ PARENT_SUBSTANCE_ID	659012FKBL
+ PARENT_SUBSTANCE_NAME	SUS SCROFA
+ DEVELOPMENTAL_STAGE	
- PART_GROUP	
+ PART	INTESTINAL MUCOSA
+ PART_LOCATION	
- FRACTION	
+ MATERIAL_TYPE	POLYSACCHARIDE
+ FRACTION	HEPARIN
+ COMMENTS	